THEORETICAL & APPLIED MECHANICS LETTERS **2**, 022003 (2012)

Simulation of flow through porous anode in MFC at higher power density

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(Received 29 November 2011; accepted 10 January 2012; published online 10 March 2012)

Abstract Microbial fuel cell (MFC) is a novel environmental friendly energy device which has received great attention due to its technology for producing electricity directly from organic or inorganic matter by using bacteria as catalyst. To date, many experiments have been carried out to achieve the maximum power output with advective flow through porous anode to the cathode in the MFC. However, the precise mechanical mechanism of flow through anode and the quantified relationship between electrode spacing and MFC performance are not yet clearly understood. It has been found experimentally that the power output can be increased apparently at certain electrode spacing configuration. Based on these available experimental data, this paper investigates the effect of spacing between electrodes, the Darcy number of porous anode and the Reynolds number on the power production performance of MFC by using lattice Boltzmann method. The numerical simulation results present that the distance between electrodes significantly influences the flow velocity and residence time of the organic matter attached to the anode in the MFC. Moreover, it is found that the Darcy number of porous anode and the Reynolds number can regulate the output efficiency of MFC. These results perform better understanding of the complex phenomena of MFC and will be helpful to optimize MFC design.
[doi:10.1063/2.1202203]

Keywords microbial fuel cell, lattice Boltzmann method, flow in porous media

Microbial fuel cell (MFC) is a novel environmental friendly energy device which converts chemical energy contained in organic compounds to electrical energy by using microorganism as a biocatalyst.[1] In the MFCs, the electrons generated by the bacteria flow from the porous anode to the cathode by the external circuit. The electrons typically combine with protons and oxygen to form water on the cathode. To date, the MFCs have received great attention due to their potential applications in many fields, such as biosensors, bio-robots, bio-catalyzed H_2, and renewable energy generation.[2–4] In addition, one of the main applications for MFCs is the wastewater treatment, since it is possible to simultaneously harvest much electricity while treating the wastewater.[5–7]

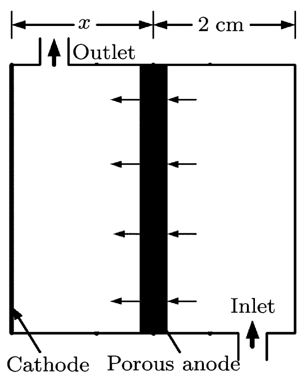

Fig. 1. Schematic view of the 2D MFC model.

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Practical applications for wastewater treatment require continuous flow operation, and many new types of systems are being proposed for continuous operation. Liu et al.[8] got a maximum power density of 26 mW/m^2 by using domestic wastewater in a single-chamber system. Min et al.[9] achieved a maximum power density of 212 mW/m^2 with glucose and 72 mW/m^2 with wastewater in a continuous flow mode by laying the electrodes on each side of the polymeric proton exchange membrane (PEM). Recently, it has been found that the maximum power output by an air-driven cathode MFC for glucose and domestic wastewater would increase when the PEM was removed and the reactor was operated under a continuous advective flow condition.[10] Moreover, it has been shown that the MFC performance was related to the spacing between the cathode and porous anode. When the electrodes distance was decreased from 3 to 1 cm, the maximum power density of MFC would increase from 826 to 1 540 mW/m^2. Although the experimental phenomenon is clear, the precise mechanical mechanism of fluid in the MFC and the influence of characters of electrodes on MFC performance are not yet clearly understood. Therefore, the objective of this paper is to numerically investigate the effect of spacing between electrodes, the Darcy number of porous anode material and the Reynolds number for flow velocity on power output performance in a two-dimensional (2D) MFC model with advective flow through the anode toward the cathode. As a computational fluid dynamic method, the lattice Boltzmann method is an effective and efficient numerical scheme for simulating fluid flows

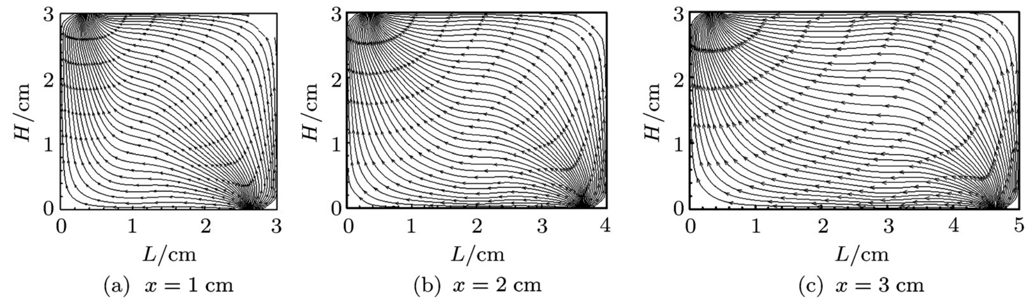

Fig. 2. Streamlines in the MFC.

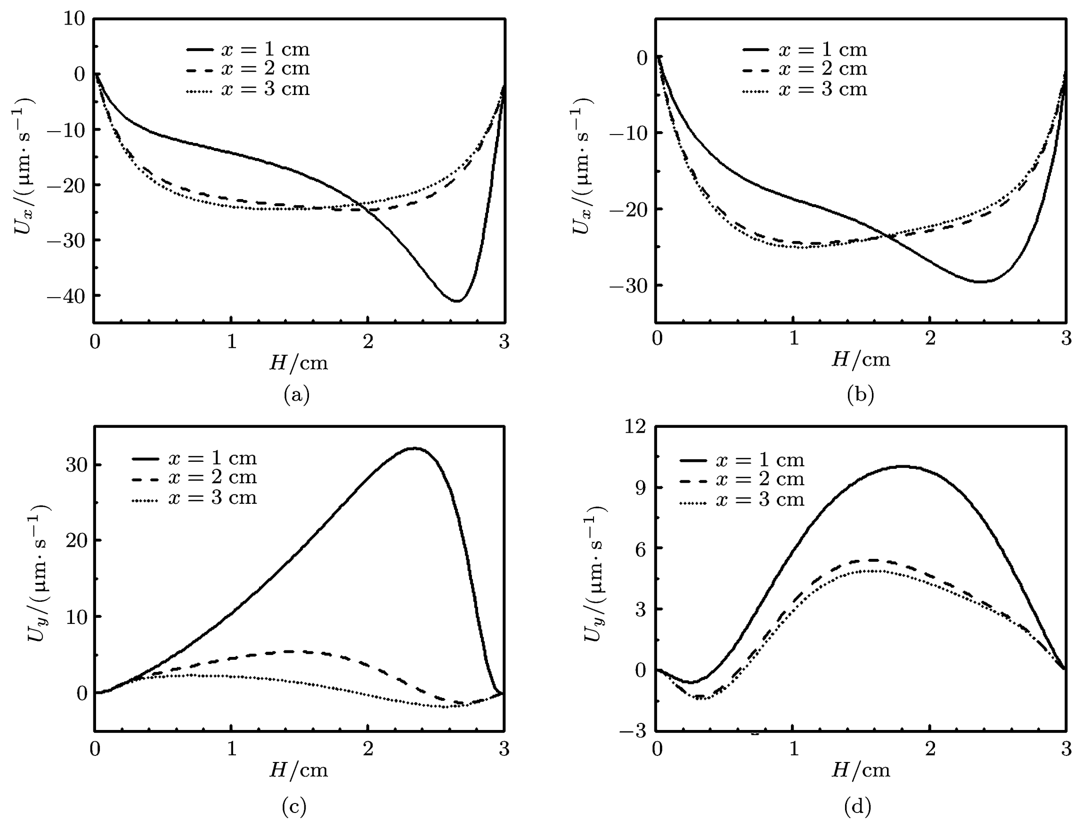

Fig. 3. Comparison of velocity distribution at both sides of porous anode for different spacing between electrodes. (a) and (c): Left side of the anode. (b) and (d): Right side of the anode.

in porous media[11] and isothermal incompressible flow through porous media[12] to analyze the performance of the MFC.

The schematic view of the 2D MFC model is shown in Fig. 1. The porous anode is fixed at 2 cm away from the entrance wall. The spacing between the anode and cathode is varied to study the effect of the electrode distance on the MFC performance. The incompressible leachate in garbage enters the MFC from the inlet and passes through the porous anode and finally leaves from outlet.

The governing equations of the Navier-Stokes model for fluid in porous medium are

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \left(\frac{\boldsymbol{u}}{\varepsilon} \right) = -\nabla(\varepsilon p) + \upsilon_{\mathrm{e}} \nabla^2 \boldsymbol{u} + \boldsymbol{F}, \tag{2}$$

where $\boldsymbol{u}$ is the volume-averaged velocity, p is the pressure, ε is the porosity of the porous media, υ_{e} is the effective viscosity determined by $\upsilon_{\mathrm{e}} = c_s^2(\tau - 0.5)\Delta t$, and $\boldsymbol{F}$ represents the total force given by

$$\boldsymbol{F} = -\frac{\varepsilon \upsilon}{K} \boldsymbol{u} - \frac{\varepsilon F_{\varepsilon}}{\sqrt{K}} \left| \boldsymbol{u} \right| \boldsymbol{u} + \varepsilon \boldsymbol{G}, \tag{3}$$

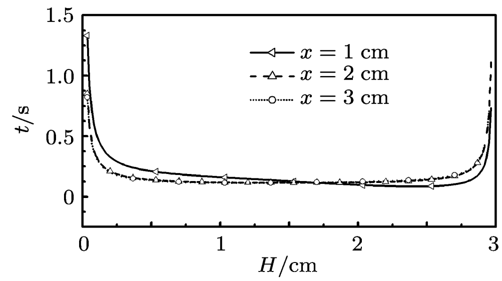

Fig. 4. Comparison of the distribution of residence time for different spacing between electrodes.

where υ is the kinematic viscosity of the fluid, and $\boldsymbol{G}$ is the body force. The geometric function F_ε and the permeability K can be expressed as[13]

$$F_\varepsilon = \frac{1.75}{\sqrt{150\varepsilon^3}}, \quad K = \frac{\varepsilon^3 d_p^2}{150(1-\varepsilon)^2}, \tag{4}$$

where d_p is the diameter of the solid particles.

The liquid flow governed by Eqs. (1) and (2) is characterized by three non-dimensional parameters: Darcy number Da, viscosity ratio J, and Reynolds number Re, which are defined as: $Da = K/L^2$, $J = \upsilon_e/\upsilon$, and $Re = LU/\upsilon$, respectively, where U is the velocity and L is the characteristic length.

The lattice Boltzmann equation for porous flow can be expressed as

$$\overline{f_i}(\boldsymbol{x} + \boldsymbol{e}_i\Delta t, t + \Delta t) = \overline{f_i}(\boldsymbol{x}, t) - \frac{\overline{f_i}(\boldsymbol{x}, t) - \overline{f_i}^{\mathrm{eq}}(\boldsymbol{x}, t)}{\tau} + F_i\Delta t, \tag{5}$$

where $\overline{f_i}(\boldsymbol{x}, t)$ is the volume-average density distribution function for the particle with velocity $\boldsymbol{e}_i$ at position $\boldsymbol{x}$ and time t, τ is the non-dimensional relaxation time, and Δt is the time increment. The volume-average equilibrium distribution function $\overline{f_i}^{\mathrm{eq}}(\boldsymbol{x}, t)$ is defined as

$$\overline{f_i}^{\mathrm{eq}} = \omega_i\rho\left[1 + \frac{\boldsymbol{e}\cdot\boldsymbol{u}}{c_s^2} + \frac{\boldsymbol{uu} : (\boldsymbol{e}_i\boldsymbol{e}_i - c_s^2\boldsymbol{I})}{2\varepsilon c_s^4}\right], \tag{6}$$

where ω_i is the weight with the values $\omega_0 = 4/9$, $\omega_i = 1/9$ for $i = 1$–4, and $\omega_i = 1/36$ for $i = 5$–8. Here, $c = \Delta x/\Delta t$ is the lattice speed with $c_s = c/\sqrt{3}$.

The force term F_i in Eq. (5) that accounts for the total force due to the presence of the porous medium and buoyancy effect is given by

$$F_i = \omega_i\rho\left(1 - \frac{1}{2\tau}\right)\left[\frac{\boldsymbol{e}_i\cdot\boldsymbol{F}}{c_s^2} + \frac{\boldsymbol{uF} : (\boldsymbol{e}_i\cdot\boldsymbol{e}_i - c_s^2\boldsymbol{I})}{\varepsilon c_s^4}\right]. \tag{7}$$

Based on the D2Q9 lattice Boltzmann model, the discrete velocities $\boldsymbol{e}_i$ are

$$\boldsymbol{e}_i = \begin{cases} 0, \quad i = 0, \\ \left[\cos\left(\dfrac{i-1}{2}\pi\right), \sin\left(\dfrac{i-1}{2}\pi\right)\right], \\ \qquad i = 1-4, \\ \sqrt{2}\left[\cos\left(\dfrac{2i-1}{4}\pi\right), \sin\left(\dfrac{2i-1}{4}\pi\right)\right], \\ \qquad i = 5-8. \end{cases} \tag{8}$$

The volume-averaged density and velocity are defined as

$$\rho = \sum_i f_i, \quad \boldsymbol{u} = \boldsymbol{v}\Big/\left(c_0 + \sqrt{c_0^2 + c_1|\boldsymbol{v}|}\right). \tag{9}$$

The three parameters c_0, c_1, and $\boldsymbol{v}$ in Eq. (9) are given by

$$c_0 = \frac{1}{2}\left(1 + \varepsilon\frac{\upsilon\Delta t}{2K}\right), \quad c_1 = \varepsilon\frac{F_\varepsilon\Delta t}{2\sqrt{K}},$$
$$\boldsymbol{v} = \sum_i \overline{f_i}\frac{\boldsymbol{e}_i}{\rho} + \frac{\Delta t}{2}\varepsilon\boldsymbol{G}. \tag{10}$$

The porous anode is fixed at 2 cm against the entrance wall, and the distance between the cathode and anode is varied from 1 to 3 cm. The continuous leachate flows through the porous anode to the cathode. The calculations are carried out to study the effect of the spacing between electrodes under advective flow conditions.

Figure 2 shows the streamlines in the MFC at $x = 1$ to 3 cm. Figure 3 illustrates the comparison of velocity distribution along the vertical line of the both sides on porous anode for different spacing between electrodes. At $x = 1$ cm in which the power density achieved maximum in experiment, the horizontal velocity profiles on both sides are skewed toward the outlet. When we increase the spacing to $x \geq 2$ cm, the velocity profiles are almost symmetric. Simultaneously, the vertical velocities on both sides reach to the maximum at the optimized spacing $x = 1$ cm. It indicates that the higher vertical velocity would be better to enhance the power density. The comparison of the residence time for different spacing between electrodes is also shown in Fig. 4. The average time at spacing $x = 1$ cm is higher than that at spacing $x = 2$ and 3 cm. Therefore the organic substance in wastewater can be highly decomposed by the microorganisms attached to the anode. The performance of the power generation can be improved when the spacing decreases.

It is well known that wastewater across the anode reacts with the microorganisms attached to the anode. It is important to investigate the influence of the anodic characters such as surface area, surface roughness and pore volume on the performance of MFC, because the anode serves as a carrier for the microorganisms. Darcy number is an important parameter for the porous

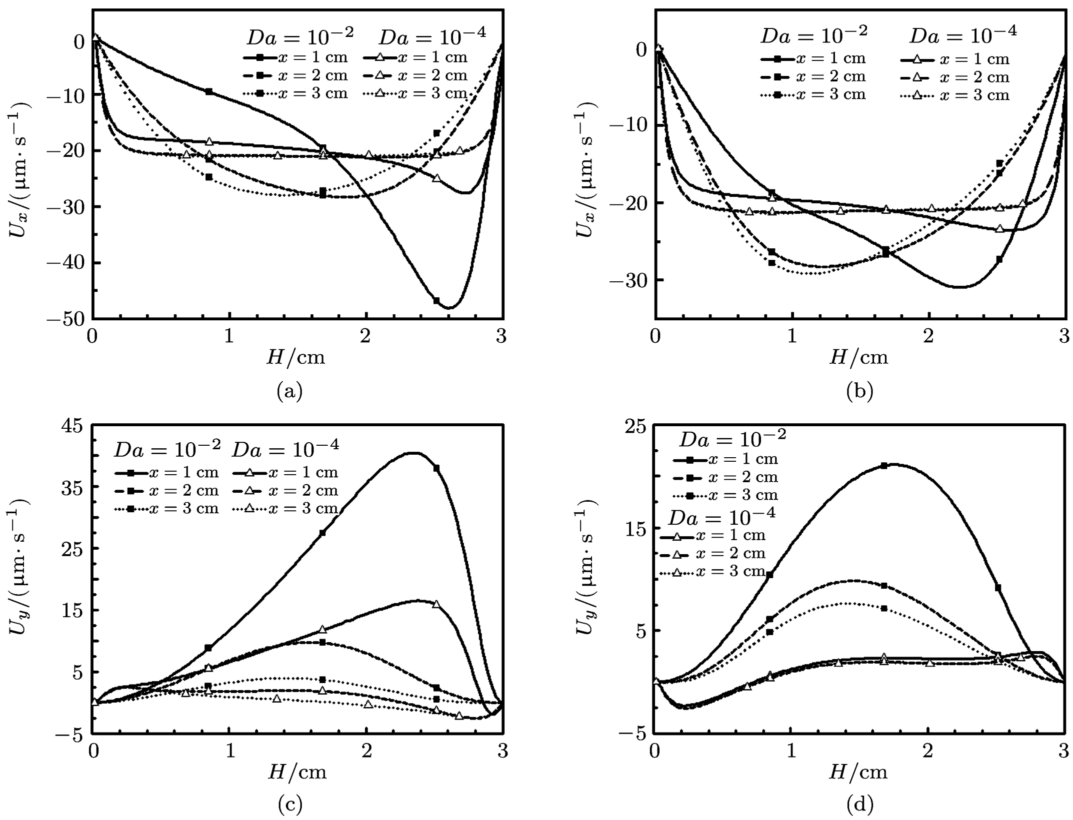

Fig. 5. Comparison of velocity distribution for different Da values at both sides of porous anode for different spacing between electrodes. (a) and (c): Left side of the anode. (b) and (d): Right side of the anode.

media.[13,14] The higher reacting efficiency in the anode will cost much more residence time. The inlet velocity will be controlled at a certain flow rate to obtain the maximum power density. Therefore the Reynolds number for flow velocity is a significant parameter. The MFC can be optimized if we can design a porous anode according to the appropriate Darcy number and select a fixed flow rate according to the appropriate Reynolds number.

Figure 5 shows the comparison of velocity distribution for different Da values at both sides of porous anode with the different electrode spacing. Obviously, the velocity profile changes significantly at higher Darcy number due to the lower flow resistance, and the velocity profile skews toward the top wall. At lower Darcy number, the velocity is almost symmetric and flat due to the higher flow resistance. At higher Darcy number $Da = 10^{-2}$, the velocity profile is sensitive to the spacing, i.e., the velocity profiles alter greatly at spacing $x = 1$ cm. At lower Darcy number $Da = 10^{-4}$–10^{-3}, the velocity profile is insensitive to the spacing, and they are almost unchanged with varied spacing $x = 1$–3 cm. When the Darcy number is too small, there is little observable effects of the electrode spacing. The flow would be plugged due to the smaller pore sizes of the anode materials. The power output would not be improved obviously by altering the electrode spacing. The effect of Darcy number must be considered in explaining the continuous-flow systems.

Figure 6 presents the comparison of velocity distribution for different Re values at both sides of porous anode with the electrode spacing $x = 1$ cm. It is shown that with the lower Re values, the velocities are almost unchanged along the porous anode side. With the higher Re values, the velocities are changed significantly at the top of the porous anode side (Figs. 6(a), 6(b) and 6(c)) and are almost symmetric in Fig. 6(d). The decomposed reaction in the anode is efficient with the lower velocity. Consequently, we can choose the appropriate Reynolds number to get a high power output.

The wastewater flow through the anode toward the cathode in MFC is simulated by the lattice Boltzmann method. The simulation results lead to the following conclusions:

(1) The performance of MFCs is related to the spacing between cathode and porous anode. The maximum power density is increased when the spacing is decreased from 3 to 1 cm under conditions of advective flow.

(2) The effect of Darcy number on the performance of MFCs must be considered when power output is improved by decreasing the electrode spacing. The MFCs can be optimized by selecting an appropriate Darcy number of the porous anode.

(3) When the electrode spacing is fixed at 1 cm, the

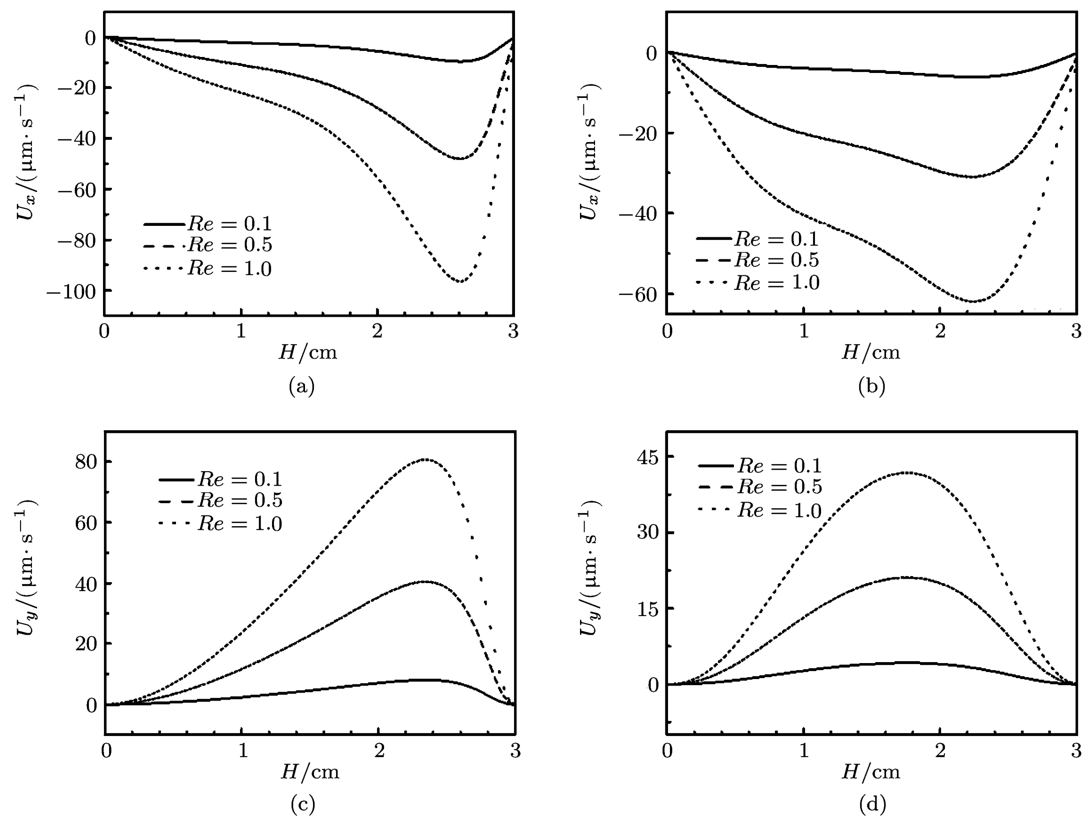

Fig. 6. Comparison of velocity distribution for different Re values at both sides of porous anode for the spacing between electrodes $x = 1$ cm. (a) and (c): Left side of the anode. (b) and (d): Right side of the anode.

velocity profile can also be influenced by the Reynolds number. Therefore, the significant parameter Reynolds number for inlet velocity can be controlled at a certain flow rate to get the maximum power density.

This work was supported by the National Natural Science Foundation of China (10932010, 10972208 and 11072220).

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